

Structure and energetics of Ga/Si(112): Adsorbate-induced "planarization" of a high-index substrate

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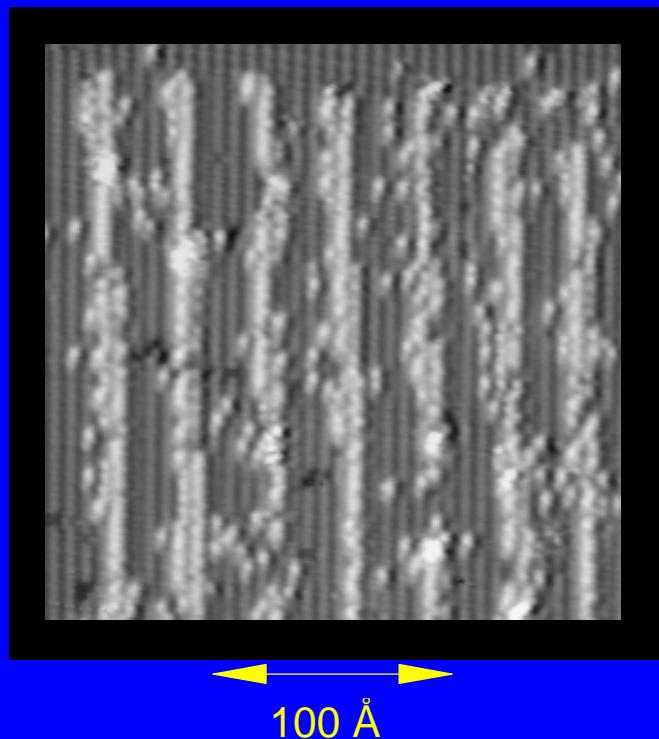
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Atomic "wires"

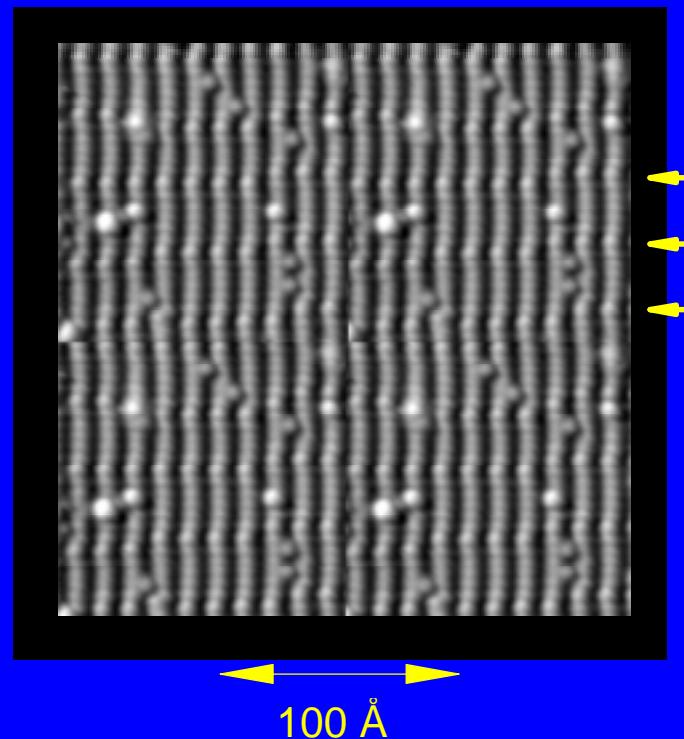
STM lithography of H/Si(001)

J.W. Lyding et al., *Appl. Phys. Lett.* 64, 2010 (1994)



- Line width = 1-2 atoms
- Line spacing = 30 Å

Ga adsorption on Si(112)



- Line width = 1 atom
- Line spacing = 9 Å
- Quasiperiodic defects?

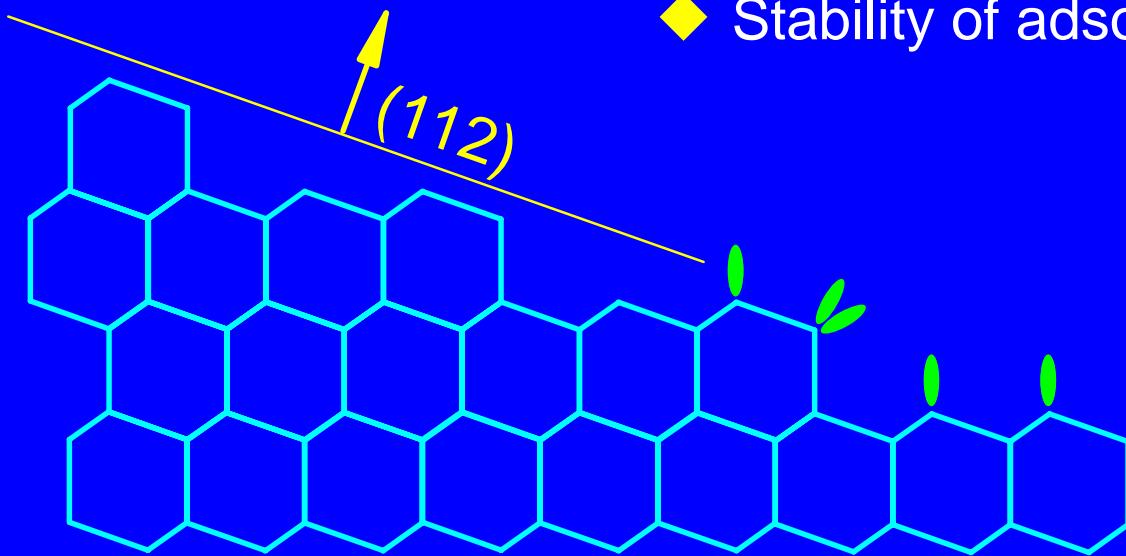
Preliminaries

Clean Si(112) surface

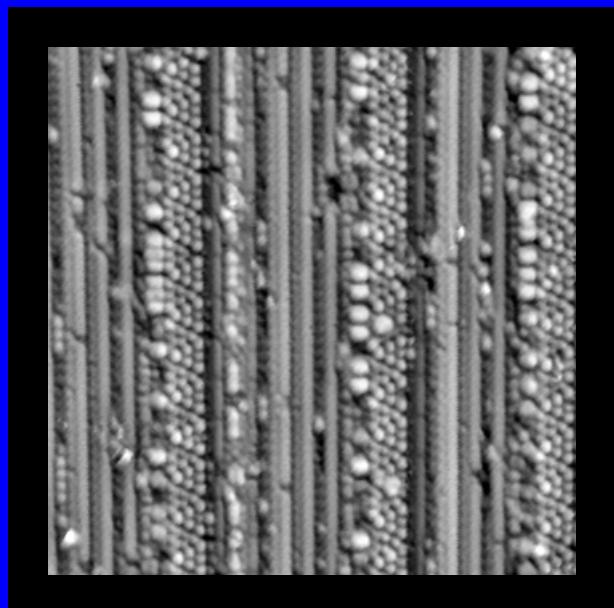
- ◆ Ideal: terrace plus step
- ◆ Stability of clean surface?

Si(112) substrate plus Ga adsorbate

- ◆ Step-edge vs. terrace adsorption
- ◆ Stability of adsorbed substrate?



Clean Si(112) surface



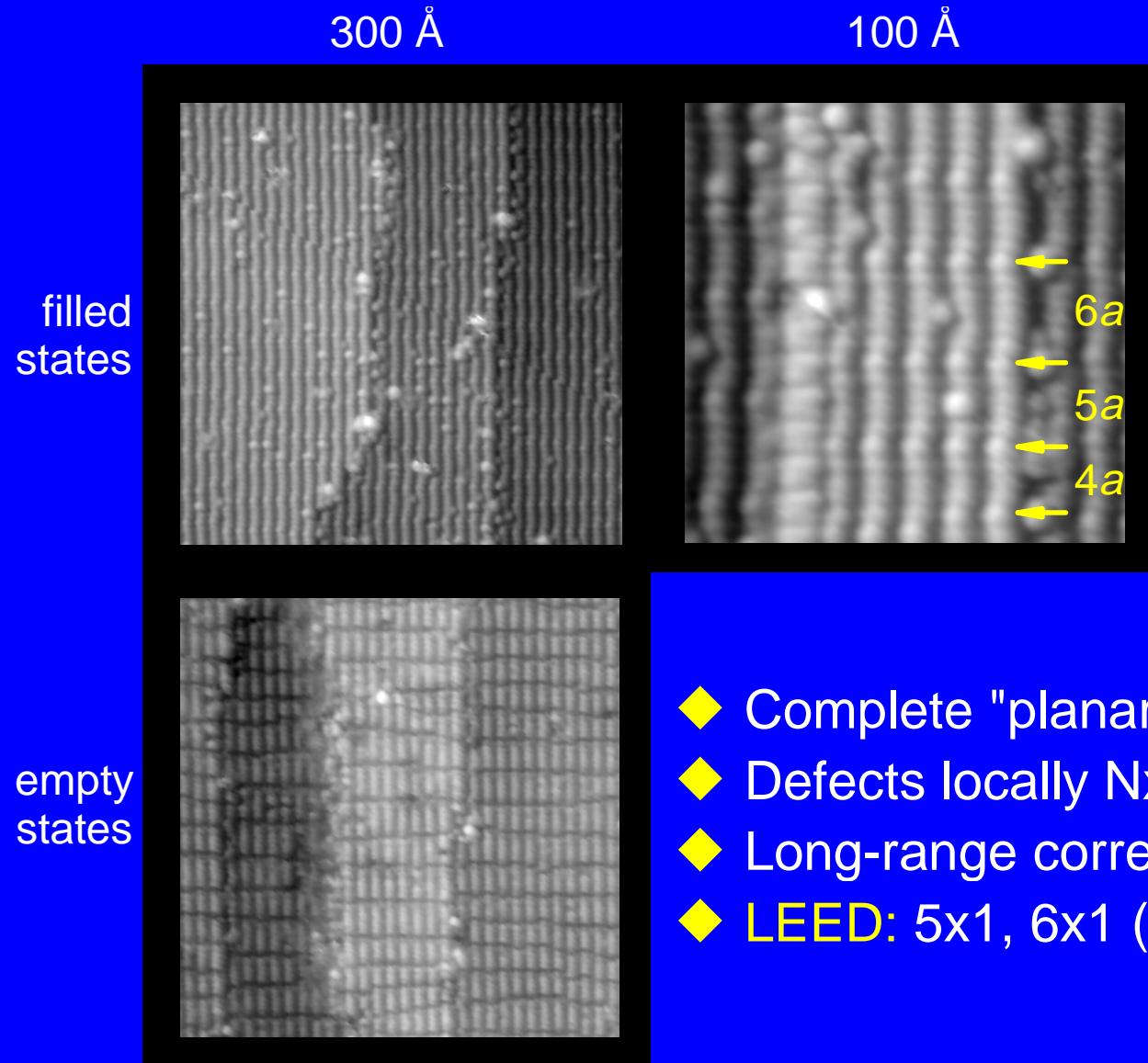
100 Å

A.A. Baski and L.J. Whitman, PRL 74, 956 (1995)

- ◆ Sawtooth "grooved" surface
- ◆ Facets: (337) and (111) 7×7
- ◆ Quasiperiodic, ~ 100 Å "period"

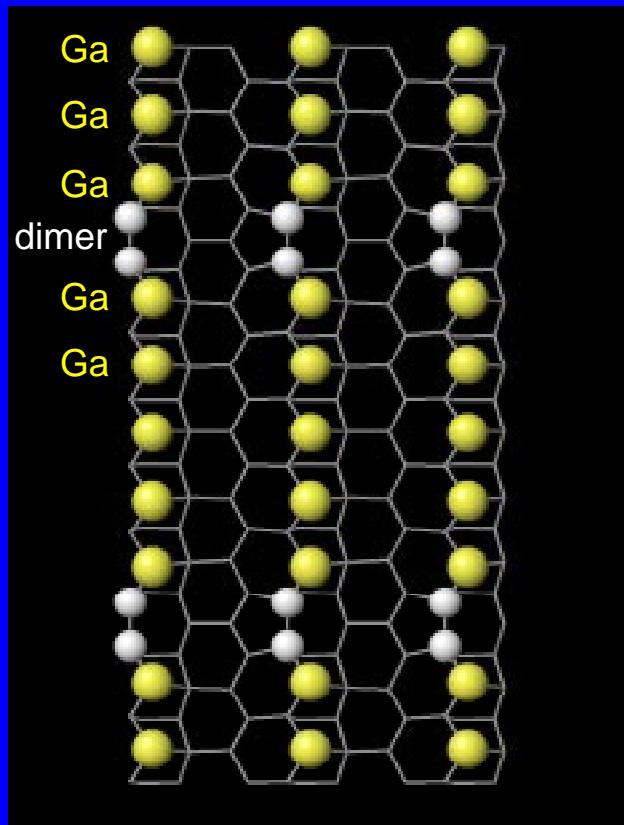
Morphology in presence of Ga adsorbates?

Ga/Si(112) reconstruction



- ◆ Complete "planarization"
- ◆ Defects locally $N \times 1$ ($N=4,5,6,7$)
- ◆ Long-range correlation
- ◆ LEED: 5×1 , 6×1 (Jung et al.)

Reconstruction model & theory

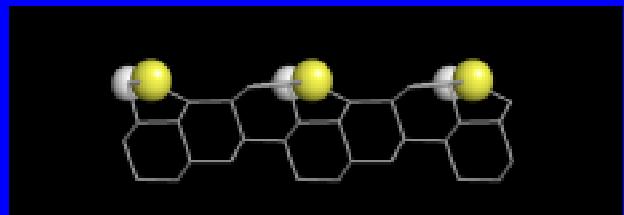


◆ Ga adsorbed at Si(112) step edge

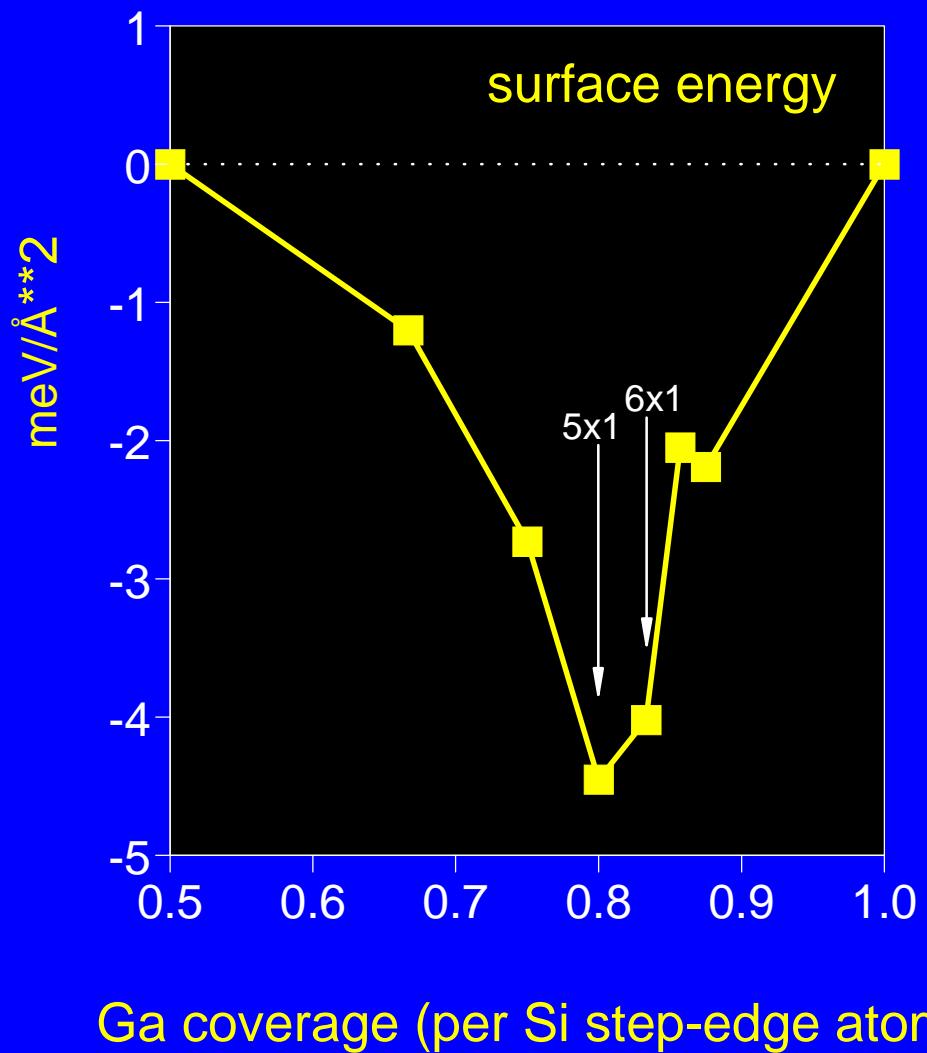
- ◆ Angle-resolved Auger spectroscopy
J.E. Yater et al., Phys. Rev. B 51, 7365 (1995)

◆ Nx1 reconstructions, N=1,2,...,8

- ◆ every Nth Ga atom missing
- ◆ unbonded Si atoms rebond to form dimer
T.M. Jung et al., J. Vac. Sci. Tech. A 12, 1838 (1994)



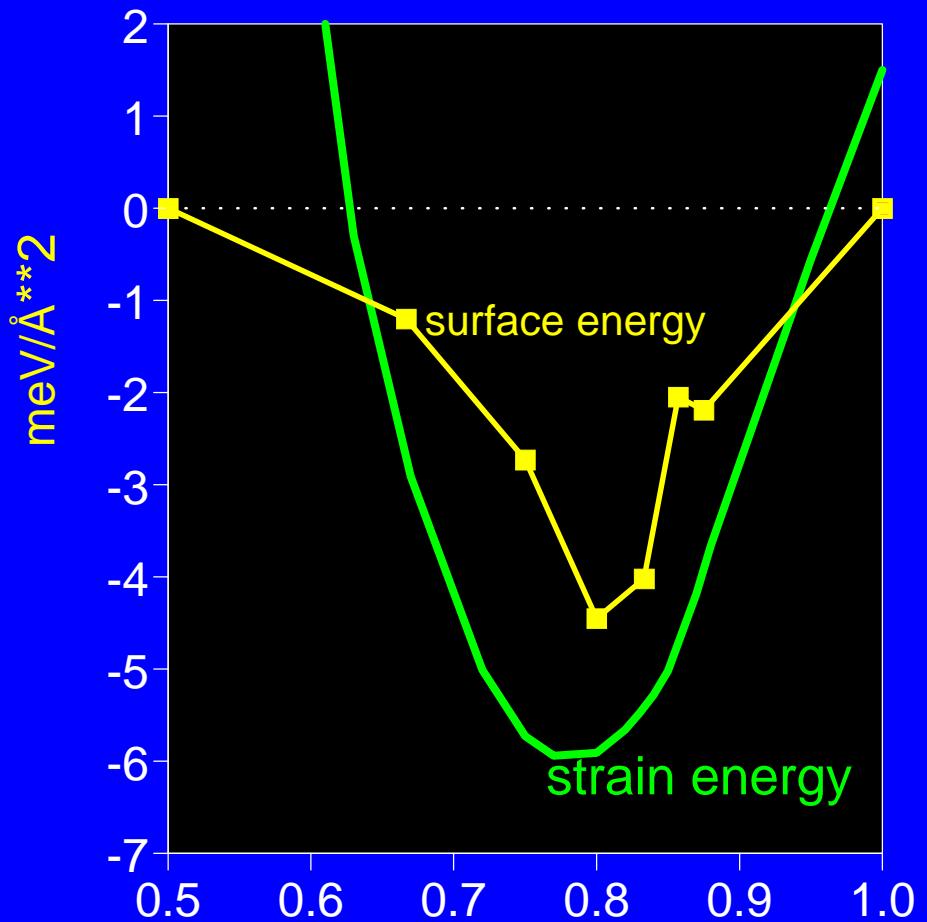
Reconstruction energy vs. N



- ◆ First-principles theory (LDA)
 - ◆ ab initio pseudopotentials
 - ◆ planewave basis, $E_{\text{cut}} = 8 \text{ Ry}$
 - ◆ generalized gradient approximation
- ◆ Slab geometry, 8 Si layers
- ◆ Complete structural relaxation

Surface energy
 $\gamma = A^{-1}(E_t - N_{\text{Ga}}E_{\text{Ga}} - N_{\text{Si}}E_{\text{Si}})$
"Energy to create surface from bulk"

Reconstruction energy: a simple model



Ga coverage (per Si step-edge atom)

- ◆ Bond strains at (112) step edge
 - ◆ Si-Si dimer: small N \Rightarrow large strain
 - ◆ Ga-Si chain: large N \Rightarrow large strain
 - ◆ Competition \Rightarrow intermediate N
- ◆ One-parameter Ansatz for $\gamma(N)$
 - ◆ $\gamma(\text{Si-Si}) = \text{Stillinger-Weber}$
 - ◆ $\gamma(\text{Ga-Si}) = \text{Constant} \times (\text{strain})^2$
 - ◆ Ignore: dangling bonds, stress, etc.

Theoretical STM images

- First-principles theory \Rightarrow geometry and wavefunctions
- Wavefunctions \Rightarrow local density of states (LDOS):

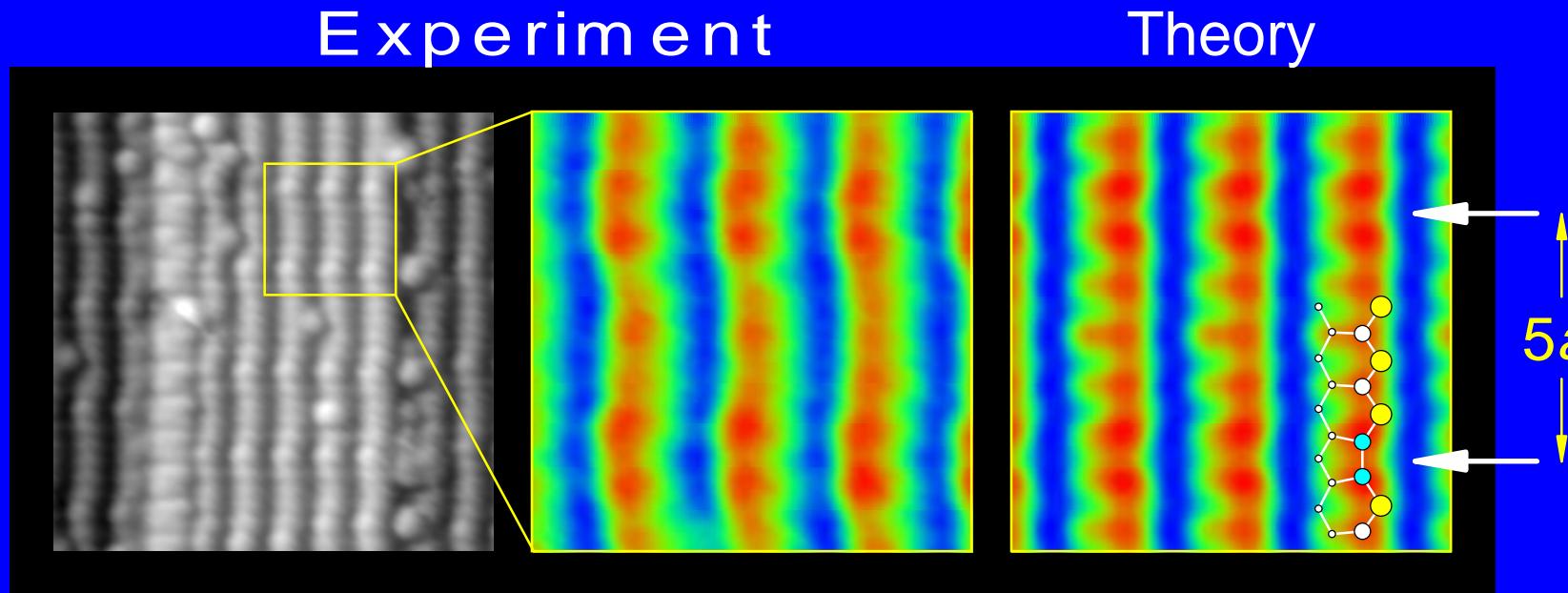
$$\rho(r,\varepsilon) = \sum_{nk} |\Psi_{nk}(r)|^2 \delta(\varepsilon - \varepsilon_{nk})$$

- LDOS \Rightarrow energy-integrated LDOS:

$$q(r) = \int \rho(r,\varepsilon) d\varepsilon$$

- Surface of constant $q(r)$ \Rightarrow constant-current STM topography

STM comparison



- Theory explains..
- ◆ Existence of defects on Ga/Si(112)
 - ◆ Ga vacancies + rebonded Si dimers
 - ◆ optimal separation of vacancies = $5a$, $6a$
 - ◆ Topography of STM images
 - ◆ double spots \Leftrightarrow two dimer atoms
 - ◆ difference in spot heights \Leftrightarrow dimer gap state

Credits

Software

FHI96MD, M. Bockstedte, A. Kley, and M. Scheffler, CPC 1997

Additional software

PLANEWAVE, M.P. Teter, M.C. Payne, and D.C. Allan, PRB 1989

Hardware

DoD MSRC's: Maui and Wright-Patterson AFB

Funding

Office of Naval Research